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Published in:
Physics in Medicine and Biology

DOI:
10.1088/0031-9155/38/9/013

Phys. Med. Biol. **38** (1993) 1343–1350. Printed in the UK

Low-degree polynomial phase-functions with high g-value

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Received 17 March 1993

Abstract. In an attempt to construct an analytic theory of anisotropic random flight, the need has arisen to construct phase-functions for which the expansion in spherical harmonics has only a limited number of terms, but which have a high value for the asymmetry parameter g. We describe the procedure to find the phase-function which has a maximum value of g for given N, where N is the number of spherical components of the phase-function. It appears that in order to attain $g = 0.9$, one needs a phase-function composed of at least nine spherical components, or equivalently a polynomial of degree nine.

1. Introduction

The mathematical description of the propagation of light in biological tissues is usually based on diffusion theory (Farrell *et al* 1992, Patterson *et al* 1991, Groenhuis *et al* 1983) which has its limitations. Analytical random-walk theory is a promising alternative to diffusion theory (Gandjbakhche *et al* 1992), if one is interested in the behaviour of short pathlengths, near boundaries and sources etc.

Although scattering in biological tissues is often strongly peaked in the forward direction (Flock *et al* 1987), the usual approach is to perform calculations based on isotropic random-walk theory and take anisotropy into account by the use of suitable scaling laws (Wyman and Patterson 1988). A more complete theory of anisotropic random walk requires the inclusion of higher moments of the angular probability distribution, or phase-function (Van De Hulst 1980). It is then important to know how, given a fixed number of terms in the Legendre expansion of the phase-function, one can construct the most sharply peaked phase-function.

2. Method

In accordance with the above, we write the phase-function in the form

$$f(\cos\vartheta) = \sum_{l=0}^{N} a_l P_l(\cos\vartheta) \tag{1}$$

where $P_l(\cos\vartheta)$ is the Legendre polynomial of order l. Because $f(\cos\vartheta)$ is a probability density, it must be normalized and non-negative for all scattering angles. In terms of the variable $u = \cos\vartheta$, the usual normalization condition is (Van De Hulst 1980)

$$\tfrac{1}{2}\int_{-1}^{1} f(u)\,\mathrm{d}u = 1 \tag{2}$$

0031-9155/93/091343+08\$07.50

and non-negativity reads

$$f(u) \geqslant 0 \qquad -1 \leqslant u \leqslant 1. \tag{3}$$

The mean scattering cosine or g-value is (Van De Hulst 1980)

$$g = \tfrac{1}{2}\int_{-1}^{1} f(u)u\,\mathrm{d}u. \tag{4}$$

Thus, our problem is: given a polynomial of fixed degree N, maximize the value of g in equation (4), subject to conditions (2) and (3). The normalization condition (2) can always be fulfilled by simply dividing by the norm, but non-negativity (3) is more difficult to ensure. Things are most simple for even N, so that we shall treat this case first.

We thus write

$$f(u) = A(u)A^*(u) \tag{5}$$

where $A(u)$ is a polynomial of degree $N/2$.

Define the space S_m as the $(m+1)$-dimensional space containing all polynomials of degree at most m, endowed with the scalar product

$$\langle A(u)|B(u)\rangle = \int_{-1}^{1} A^*(u)B(u)\,\mathrm{d}u. \tag{6}$$

In S_m, we can choose an orthonormal basis by the first m (including zero) normalized Legendre polynomials

$$\tilde{P}_i(u) = P_i(u)\sqrt{i+\tfrac{1}{2}} \tag{7}$$

so that $\langle \tilde{P}_i|\tilde{P}_j\rangle = \delta_{i,j}$. These polynomials satisfy the recursion relation

$$u\tilde{P}_i(u) = [(i+1)/\sqrt{(2i+1)(2i+3)}]\tilde{P}_{i+1}(u) + [i/\sqrt{(2i+1)(2i-1)}]\tilde{P}_{i-1}(u) \tag{8}$$

which can be derived from the conventional relation (Abramowitz and Stegun 1964)

$$(n+1)P_{n+1}(u) = (2n+1)uP_n(u) - nP_{n-1}(u). \tag{9}$$

If we define the operator U as multiplication by the function u, we can use equation (8) to deduce a matrix representation for U in S_m; e.g. in S_3 we have

$$U = \begin{pmatrix} 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{3\cdot5}} & 0 \\ 0 & \frac{2}{\sqrt{3\cdot5}} & 0 & \frac{3}{\sqrt{5\cdot7}} \\ 0 & 0 & \frac{3}{\sqrt{5\cdot7}} & 0 \end{pmatrix} \tag{10}$$

We can now reformulate our problem in terms of $A(u)$, namely, find the polynomial $A(u)$ of degree $\frac{1}{2}N$ for which

$$\langle A|U|A\rangle/\langle A|A\rangle = g \tag{11}$$

is a maximum, subject to no further conditions. $UA(u)$ is a polynomial of degree $\frac{1}{2}N+1$, but the component which is not in $S_{N/2}$ will vanish on taking the inner product, so we may limit the problem to $S_{N/2}$. The functional in (11) is simply a Rayleigh quotient, so by the use of the Lagrange multiplier λ it can easily be shown (Mathews and Walker 1970) that maximizing this functional is equivalent to maximizing $\langle A|U|A\rangle - \lambda\langle A|A\rangle$, which, on taking the gradient with respect to $|A\rangle$, can be rewritten as the eigenvalue problem

$$U|A\rangle = \lambda|A\rangle. \tag{12}$$

Hence the problem has been reduced to finding the eigenvalues and eigenfunctions of the matrix of U in $S_{N/2}$ (like the one in equation (10)). Since U is a Hermitian operator, all eigenvalues will be real. The calculation of the eigenvalues is straightforward, and by multiplying equation (12) from the left by $\langle A|$ and comparing with equation (11), we see that the greatest eigenvalue will be equal to g.

Once the eigenvalues are known we may find the eigenfunctions as follows: suppose $A_\mu(u)$ is an eigenfunction, belonging to eigenvalue μ. We then have $(U-\mu)|A_\mu\rangle = 0$ and hence

$$\langle B|(u-\mu)A_\mu\rangle = 0 \qquad \text{for all } B \in S_{N/2}. \tag{13}$$

Therefore $(U-\mu)|A_\mu\rangle$ is in the orthogonal complement of the space $S_{N/2}$. But since $(u-\mu)A_\mu(u)$ is a polynomial of degree $\frac{1}{2}N+1$, it is also confined to the space $S_{N/2+1}$. These two conditions fix $(u-\mu)A_\mu(u)$ up to a proportionality constant

$$(u-\mu)A(u) \propto K_{N/2+1}(u) \tag{14}$$

where $K_{N/2+1}$ is a polynomial of degree $\frac{1}{2}N+1$ in the orthogonal complement of $S_{N/2}$. However, a similar argument holds for all eigenvalues. Hence $K_{N/2+1}(u)$ must be proportional to $(u-\lambda_i)$ for all $\frac{1}{2}N+1$ eigenvalues λ_i. Therefore, $K_{N/2+1}(u)$ itself is fixed up to a constant of proportionality and we may set it equal to the characteristic polynomial of the matrix of U in $S_{N/2}$

$$K_{N/2+1}(u) = (u-\lambda_1)\ldots(u-\lambda_{N/2+1}). \tag{15}$$

For the eigenfunction $A_\mu(u)$ we have from (14)

$$A_\mu(u) = \frac{K_{N/2+1}(u)}{(u-\mu)} = \prod_{\lambda_i \neq \mu}(u-\lambda_i). \tag{16}$$

Since all eigenvalues are real, so are the eigenfunctions. Thus the phase-functions, which we were looking for, are given by

$$f_{N/2}(u) = L[K_{N/2+1}(u)/(u-\lambda_{\max})]^2 \tag{17}$$

in which L is the normalization constant, given by

$$L^{-1} = \frac{1}{2}\int_{-1}^{1}[K_{N/2+1}(u)/(u-\lambda_{\max})]^2\,\mathrm{d}u \tag{18}$$

and $\lambda_{\max} = g$.

In the case of even N we can actually do slightly better, because the characteristic polynomial $\Delta_m(\lambda)$ of the $(m+1)\times(m+1)$ matrix of U in S_m, multiplied by some constant c_m, is the Legendre polynomial of degree $m+1$, $c_m\Delta_m(\lambda) = P_{m+1}(\lambda)$. To see this, expand the determinant of the matrix of $U - \lambda\mathbf{I}$ in S_m, where $\mathbf{I}$ is the $(m+1)\times(m+1)$ identity matrix. This gives the recursion relation

$$\Delta_{m+1}(\lambda) = \lambda\Delta_m(\lambda) - [m^2/(2m+1)(2m-1)]\Delta_{m-1}(\lambda). \tag{19}$$

The coefficient of λ^{m+1} in $\Delta_m(\lambda)$ is unity. The coefficient of u^{m+1} in the Legendre polynomial of degree $m+1$ is $[2(m+1)]!/2^{m+1}(m+1)!^2$. Therefore, if c_m exists, it will have this value.

If we now multiply equation (19) by c_m and try to deduce a recursion relation for $c_m\Delta_m(\lambda)$, we obtain exactly equation (9). Because we also have $c_0\Delta_0(\lambda) = P_1(\lambda)$ and $c_1\Delta_1(\lambda) = P_2(\lambda)$, the relation deduced above is valid for all m. Hence for even N, the $g_{\max}$ value is simply the greatest zero of the Legendre polynomial $P_{N/2+1}$ and the corresponding phase-function is

$$f_N(u) = LP^2_{N/2+1}(u)/(u - g_{\max})^2 \tag{20}$$

where L accounts for normalization. The zeros of the Legendre polynomials are tabulated and lie all on the real axis, between -1 and 1 (Abramowitz and Stegun 1964). So if N is even, the maximum g-value and the corresponding phase-function can be calculated without having to find eigenvalues explicitly.

If N is odd the procedure is more or less the same. Positivity must now be ensured by setting the phase-function equal to $A(u)A^*(u)V(u)$, where $V(u) = a(u+b)$ is a linear function. Because of normalization we may set $a = 1$ and because of non-negativity b must be greater than unity in any event. To find out the actual value of b we calculate the dependence of $g_{\max}$ on b

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}b}\int_{-1}^{1} A^*(u)A(u)u(u+b)\,\mathrm{d}u \Big/ \int_{-1}^{1} A^*(u)A(u)(u+b)\,\mathrm{d}u \\ = \frac{\mathrm{d}}{\mathrm{d}b}\frac{M_2 + bM_1}{M_1 + bM_0} = \frac{M_1^2 - M_0M_2}{(M_1 + bM_0)^2}\end{aligned} \tag{21}$$

where M_i denotes the ith moment of $A^*(u)A(u)$. But the right-hand side of equation (21) is always negative, since the denominator is positive and from the Cauchy–Schwarz inequality we have $|\langle u\,A|A\rangle|^2 < \langle A|A\rangle\langle u\,A|u\,A\rangle$. Hence we can choose b to be as low as is consistent with non-negativity of the resulting phase-function, which results in the value $b = 1$.

The functional to be maximized is now

$$\langle A|U(1+U)|A\rangle/\langle A|(1+U)|A\rangle = g. \tag{22}$$

Proceeding as in the above we find that this is equivalent to solving the generalized eigenproblem in $S_{N/2+1}$

$$U(1+U)|A\rangle = \lambda(1+U)|A\rangle. \tag{23}$$

The matrix representation of the operators in equation (23) is not as simple as in the case of even N, but it is easy to see that all matrices are still symmetric. The eigenvalues can

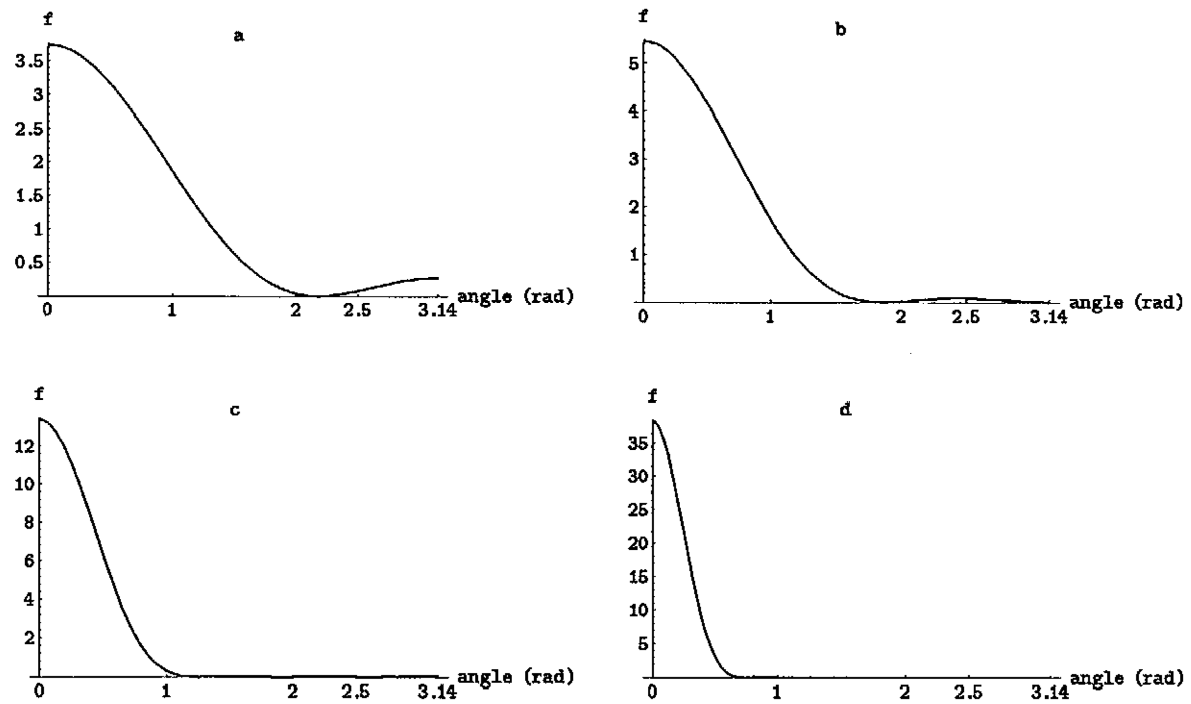

Figure 1. Plots of phase-functions with a maximum value of g for various numbers N of spherical components: (a) $N = 2$, $g = 0.58$; (b) $N = 3$, $g = 0.69$; (c) $N = 6$, $g = 0.86$; (d) $N = 12$, $g = 0.95$.

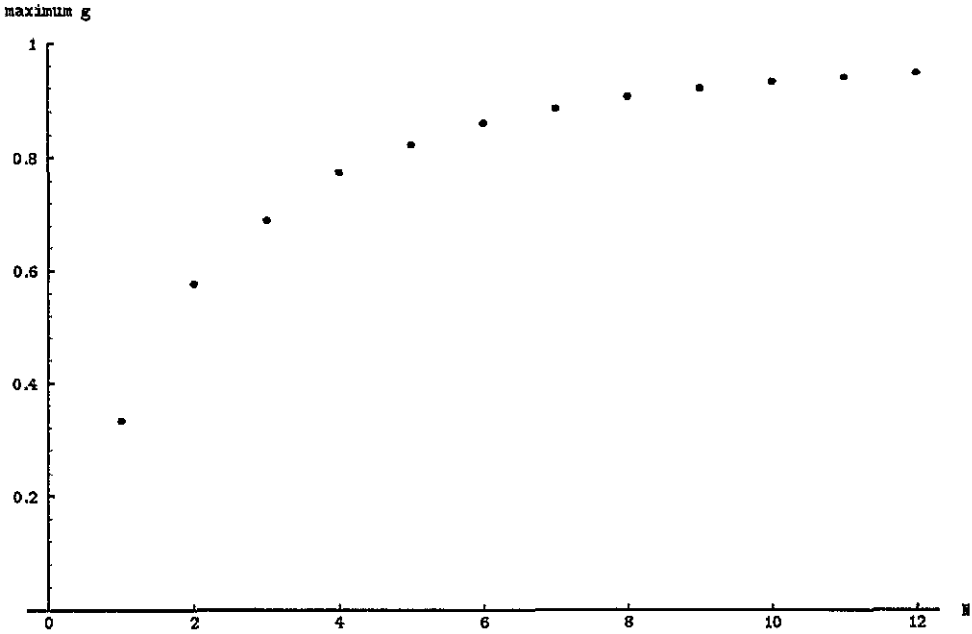

Figure 2. The maximum g-value as a function of the number N of spherical components.

be found by solving the equation $\det[U(1+U)-\lambda(1+U)]=0$ and by a similar argument to that following equation (14), it can be shown that the eigenfunctions are related to the characteristic polynomial as in equation (16). Hence the desired phase-functions are now given by

$$f_N(u) = L(1+u)[K_{N/2+1}(u)/(u-\lambda_{\max})]^2 \tag{24}$$

in which $g=\lambda_{\max}$ and L ensures normalization, as before.

If N is odd, there seems to be no simple relationship between the characteristic polynomial of U and the Legendre polynomials, so in this case, eigenvalues must be calculated explicitly. Still, this is no more complicated than solving one algebraic equation numerically.

3. Results and conclusions

We have calculated the phase-functions of polynomial degree N which maximize the value of g. For even N, they are given by equation (20) in which $P^2_{N/2+1}(u)$ is the Legendre polynomial of degree $\frac{1}{2}N+1$, $g_{\max}$ is the greatest zero of this polynomial and also the value of g, and L is the normalization constant, defined by $L^{-1}=\frac{1}{2}\int_{-1}^{1}P^2_{N/2+1}(u)/(u-g_{\max})^2\,\mathrm{d}u$. For odd N we have equation (24) in which $K_{N/2+1}(u)$ is a characteristic polynomial defined by

$$K_{N/2+1}(\lambda) = \det[\mathbf{Q}-\lambda\mathbf{R}] \tag{25}$$

in which **Q** and **R** are $(\frac{1}{2}N+1)\times(\frac{1}{2}N+1)$ matrices, defined by

$$Q_{i,j}=\int_{-1}^{1}\frac{P_i(u)P_j(u)}{\sqrt{(i+\frac{1}{2})(j+\frac{1}{2})}}u(1+u)\,\mathrm{d}u \tag{26}$$

and

$$R_{i,j}=\int_{-1}^{1}\frac{P_i(u)\,P_j(u)}{\sqrt{(i+\frac{1}{2})(j+\frac{1}{2})}}(1+u)\,\mathrm{d}u \tag{27}$$

respectively. $P_l(u)$ is the Legendre polynomial of degree l, as before. Furthermore $g_{\max}$ is the greatest zero of $K_{N/2+1}$ and this is also the maximum g-value, and L is the normalization constant, for which

$$L^{-1}=\tfrac{1}{2}\int_{-1}^{1}\frac{K_{N/2+1}^{2}(u)}{(u-g_{\max})^2}(1+u)\,\mathrm{d}u. \tag{28}$$

Table 1.

N	g	$f_N(u)$
1	0.333 33	$1+u$
2	0.577 35	$1.5(0.577\,35+u)^2$
3	0.689 90	$1.637\,67(1+u)(0.289\,90+u)^2$
4	0.774 60	$2.5u^2(0.774\,60+u)^2$
5	0.822 82	$3.0908(1+u)(u-0.181\,07)^2(0.575\,32+u)^2$
6	0.861 14	$4.9468(u-0.339\,98)^2(0.339\,98+u)^2(0.861\,14+u)^2$
7	0.885 79	$6.6783(1+u)(u-0.446\,31)^2(0.167\,18+u)^2(0.720\,48+u)^2$
8	0.906 18	$11.091(u-0.538\,47)^2u^2(0.538\,47+u)^2(0.906\,18+u)^2$
9	0.920 38	$15.935(1+u)(u-0.603\,97)^2(u-0.124\,05)^2(0.390\,93+u)^2(0.802\,93+u)^2$
10	0.932 47	$27.202(u-0.661\,21)^2(u-0.238\,62)^2(0.238\,62+u)^2(0.661\,21+u)^2(0.932\,47+u)^2$
11	0.941 37	$40.916(1+u)(u-0.703\,84)^2(u-0.326\,03)^2(0.117\,34+u)^2(0.538\,47+u)^2(0.853\,89+u)^2$
12	0.949 11	$71.312(u-0.741\,53)^2(u-0.405\,85)^2u^2(0.405\,85+u)^2(0.741\,53+u)^2(0.949\,11+u)^2$

Table 1 lists the first twelve maximum-g phase-functions, together with their g-value. A few of them have also been plotted in figures 1 and 2.

It can be concluded that in order to attain large g, one still needs polynomials of high degree, even if one uses the phase-functions with maximal g-value for a given degree, i.e. those that we calculated. For g to be 0.95, which is a typical value in soft tissues, one needs to retain over twelve terms in the Legendre expansion of the phase-function.

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